Malaysian Journal of Chemistry, 2018, Vol. 20(2), 148 - 153

Study of Thermo Physical Properties of Binary Liquid Mixtures

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Density and ultrasonic study for the binary mixtures of acetone and nitrobenzene over the entire concentration range were measured at temperatures 313 K. The experimental data was then used to calculate the compressibility and acoustic impedance, molecular free length, inverse relaxation time and excess parameters. The values of excess properties further fitted with Redlich–Kister polynomial equation to estimate the binary coefficients. The resulting excess functions were interpreted in terms of the interactions between the molecules in the binary mixtures. Results confirmed that dipole-dipole intermolecular interaction took place between acetone and nitrobenzene.

Key words: Compressibility; acoustic impedance binary mixtures; ultrasonic velocity; excess parameters

Received: March 2018; Accepted: July 2018

Ultrasonic study and its analysis for aprotic binary liquid mixtures containing polar-polar components have significant importance in understanding intermolecular interaction and strength between the component molecules as they find application in various industrial and technological processes [1]. Ultrasonic velocity and its derived acoustical parameters like adiabatic compressibility, free length, relaxation time, acoustic impedance with their excess parameters, gives important information about the molecular interactions and their strengths [1-10]. In the present paper, the variation of various parameters of binary mixtures containing nitrobenzene and acetone at 2 MHz frequency have been studied for the entire range of concentration (0-100%). Nitrobenzene is a polar molecule of benzene family different than that of ketone family of acetone. When it is mixed with acetone, the dipole-dipole bonded interaction dominates. Acetone is small sized and its linear aliphatic configuration is the important factor which mainly contributes to the volume contraction of the mixture [11]. Nitrobenzene is relatively a complex molecule. It is highly reactive even if at low temperature. Acetone being polar protic solvent is quite expected to be involved in any strong interaction with the other components of the mixture [11-17].

EXPERIMENTAL

Chemicals

In the present system of nitrobenzene+acetone binary mixture nitrobenzene is used of analytical reagent grade and is obtained from MERCK (99.99) and acetone is of HPLC grade. Both the liquids are used without further purification.

Solution Preparation

The solutions were prepared at different volume percentages of nitrobenzene in acetone in steps of 10% at room temperature (droplets of NB are mixed in acetone with increasing volume percentage). These concentrations were prepared for 5 ml solution samples at room temperature, assuming ideal mixing behavior, with an accuracy ± 0.0006 ml.

Density Measurement

The density measurements were carried out by portable digital density meter (DMA-35, Anton Paar) for pure liquids and binary mixture. This digital density meter uses the vibrating U-tube principle to calculate the density of the sample. The required quantity of the sample is approximately 2 ml. The accuracy of the instrument used is = 0.0001 g/cm^3.

Ultrasonic Velocity Measurements

The ultrasonic velocity measurements are studied using ultrasonic interferometer (Model F-05, Mittal Enterprises, New Delhi). It is single crystal interferometer operating at 2MHz fixed frequency. The sample cell of the instrument is made up of steel and is double walled; the required amount of the sample is approximately 10 cc.

Theory

The specific acoustic impedance is given by:

$$Z = U.\rho$$

where, U is the ultrasonic velocity (of the mixture), and ρ is the density of the mixture. The adiabatic compressibility is given by:

$$\beta = 1/(U^2.\rho)$$

where, 'U' and '$\circ$' are the velocity and density of liquid mixture.

The general formula for calculating the excess parameters is given below

$$A^E = A_m - (x_1 M_1 + (1 - x_1)M_2)$$

where, A^E is the excess parameter such as excess density x_1 mole fraction: and the excess parameters are fitted to the Redlich-Kister polynomial equation[8] of third order and this equation is given by:

$$A^E = x_1 x_2 \sum_{i=0}^{n} A_i (1 - 2x_2)^i$$

where, x_i is the mole fraction of the pure component 1 and 2.

RESULT AND DISCUSSION

The findings related to density, ultrasonic velocity of acetone + NB (Table 1), excess molar volume of acetone + NB (Figure 1), excess velocity of acetone + NB (Figure 2), **e**xcess compressibility of acetone + NB (Figure 3), excess acoustic impedance of acetone + NB (Figure 4), and excess molecular free length of aceton + NB (Figure 5) are all shown and discussed below.

Table 1. Density, ultrasonic velocity of acetone + NB.

Volume fraction of acetone	Density (g/cm^3)	Velocity (m/s)
0	0.852	1282
0.1	0.848	1274
0.2	0.843	1260
0.3	0.838	1256
0.4	0.830	1250
0.5	0.818	1225
0.6	0.810	1206
0.7	0.803	1175
0.8	0.800	1150
0.9	0.791	1115
1	0.782	1100

Figure 1 gives the excess molar volume of acetone + NB. As the concentration of acetone increases excess molar volume becomes positive. Positive values indicate that volume expansion takes place upon mixing due to the cross association between dissimilar molecules. Positive values also attributed to weak interaction between unlike molecules.

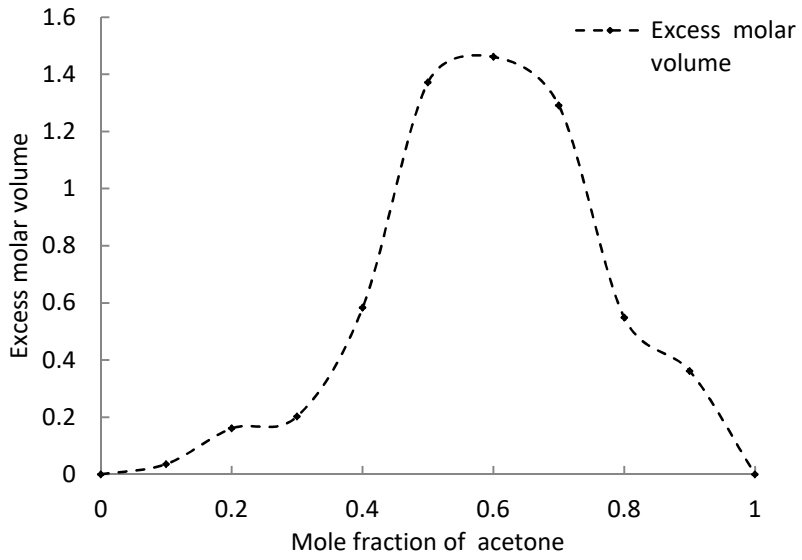

Figure 1. Excess molar volume of acetone + NB.

Figure 2. Excess velocity of acetone + NB.

As shown in Figure 2 excess velocity becomes positive as the concentration of acetone increases. Positive deviation and non-linear dependence suggest the presence of weak interaction between the components of the mixture positive excess velocity can be concluded as the formation of the structure. Weak interaction arise among the components of the mixture leading to the formation of molecular aggregates and less compact structure then sound will travel faster through the mixture by means of longitudinal waves and hence the speed of sound with respect to linear behaviour will be positive.

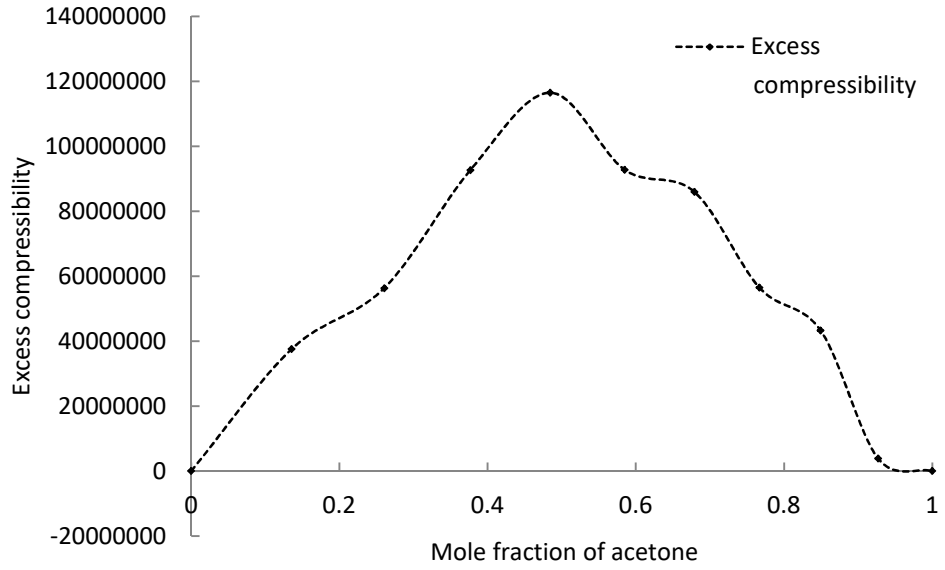

Figure 3. Excess compressibility of acetone + NB.

Figure 3 indicates excess compressibility of acetone + NB**.** The positive excess compressibility of values are due to closed packed molecules, which accounts for the existence of a weak molecular interaction between unlike molecules sign of compressibility plays the vital role in assessing the compactness due to molecular interaction in the liquid mixture through dipole-dipole interactions, leading to less compact structure making positive excess compressibility.

Positive values of acoustic impudence as shown in Figure 4 hint to the possibility of the presence of weak attractive forces between the reacting components of the mixture. Positive deviation also suggests that acetone molecules do not cooperate with NB molecules hence weak intermolecular interactions occurs between them.

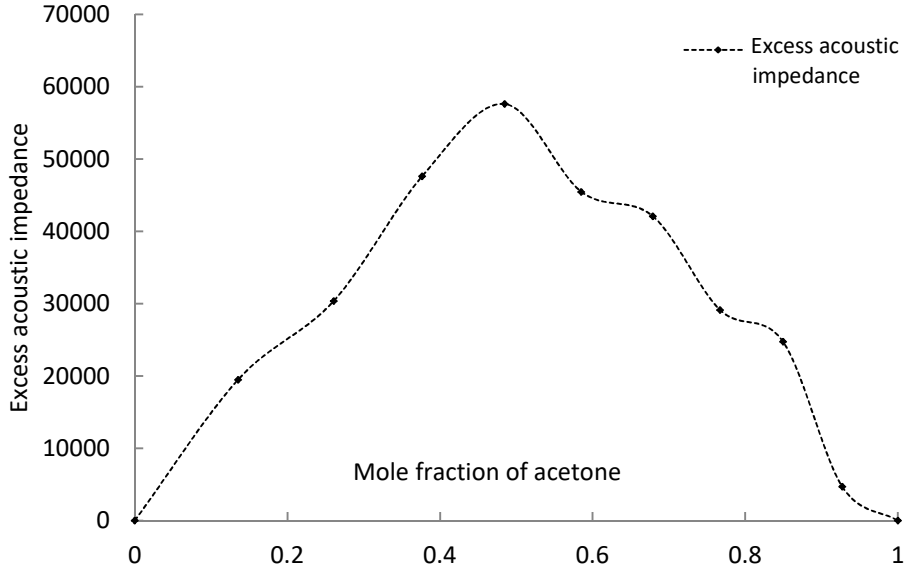

Figure 4. Excess acoustic impedance of acetone + NB.

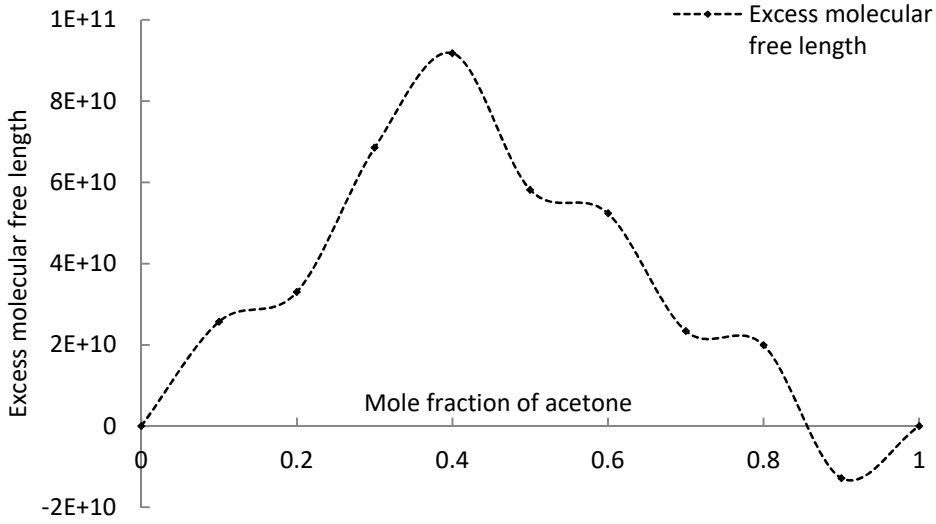

Figure 5. Excess molecular free length of aceton + NB**.**

Negative values exhibit weak interaction. The decrease in values of free length with concentration can be concluded as there is a significant interaction between two liquids. Positive values also suggest that as acetone molecules are mixed with NB molecules their intermolecular distance increased and gave rise to dipole-dipole interaction between them.

CONCLUSION

In this work, the measurement of density, ultrasonic velocity and other acoustical parameters of acetone in NB solution was studied in different concentrations at 313 K. Positive excess molar volume V_m^E values indicated the presence of weak dipole-dipole interactions. It was observed that the excess velocity values became more positive with the rise in the concentration of acetone. The experimental ultrasonic velocity data and other acoustical parameters contained valuable information regarding the solute-solvent interactions in the measurements, it could be concluded that the concentration of the acetone affected and gave rise to weak dipole-dipole interaction. Our volumetric and ultrasonic study suggested that acetone acted as structure breaker. Increase in the concentration of acetone played an important role in forming dipole-dipole interactions in the solutions.

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